POLYTECHNIQUE
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Implementation of the ELECTR module in NJOY

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2022/07/28

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Introduction

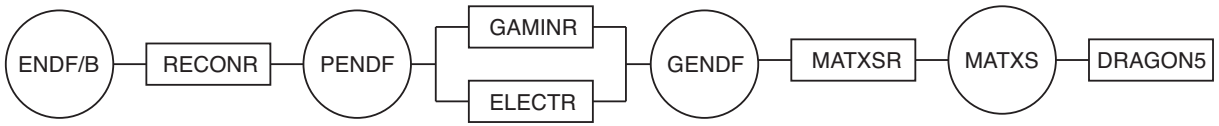
- There in a need for multigroup photoatomic and electroatomic nuclear data in many fields of engineering and science.
- In medical applications, the state-of-the-art is a Boltzmann-Fokker-Planck (BFP) solution based on the Acuros® discrete ordinates code:
  - Integrated into the Eclipse distributed calculation framework (DCF)
  - Based on CEPXS-generated multigroup cross sections (1989).
- After 30 years, there is a need for an alternative multigroup approach:
  - Use evaluated cross sections in ENDF/B or GND format, such as EPICS2017:
    - photoatomic interactions (EPDL)
    - electroatomic interactions (EEDL)
    - atomic relaxation (EADL).
  - Develop an Open-Source solution.

Introduction

- We propose a solution integrated in the NJOY processing tool:
  - Write a new processing module named ELECTR for producing multigroup electroatomic cross sections, including gamma production sets

    CEPXS mode — Use feed functions from CEPXS (restricted version)
    ENDF mode — Use feed functions adapted to the EPICS evaluation (Open Source version).

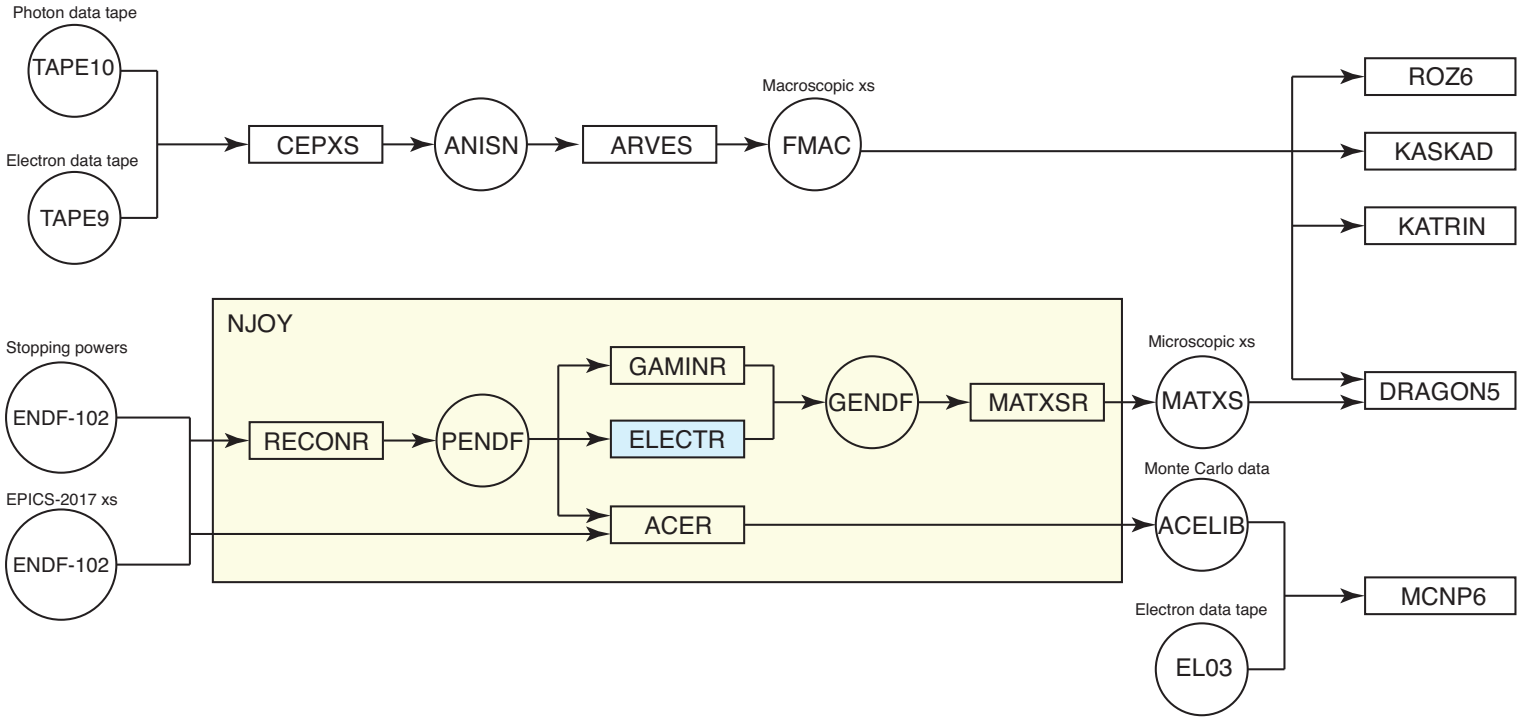
  - Update the existing GAMINR module for including electron and positron production sets
  - Update the existing MATXSR module for processing the new MT reactions.
- Update the DRAGON5 code for accepting the photoatomic and electroatomic coupled MATXS files generated with the updated system:



  - MATXS files contain microscopic cross section data.
- Validation of the CEPXS mode of the updated system will be presented in the next talk.
  - A programming issue remains to be corrected in the ENDF mode.

Coupled sets

- The ELECTR module is a new module developed in the NJOY-2012 environment by Polytechnique Montréal

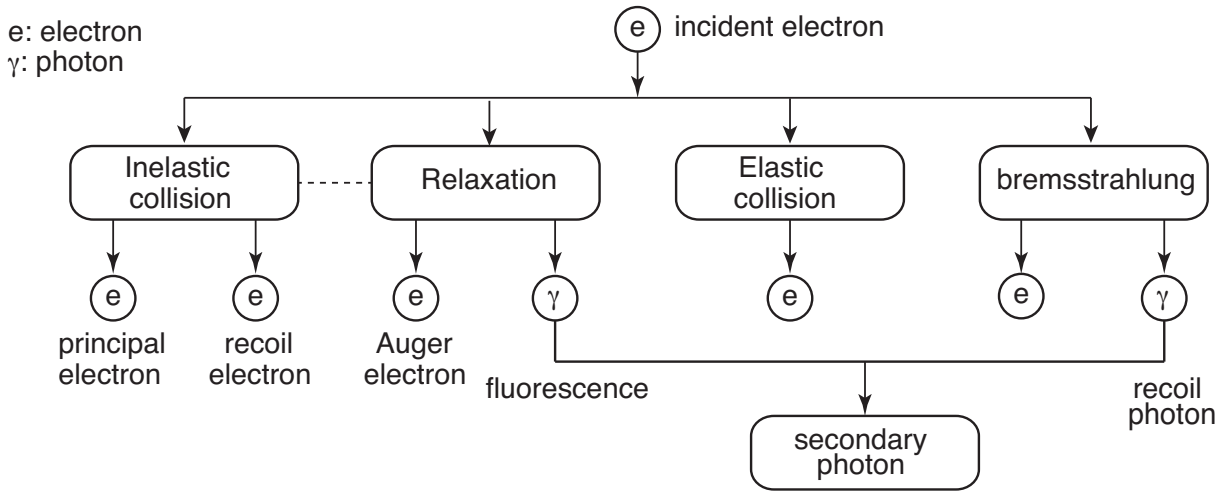


Coupled sets

- Electroatomic cross section data is generated using the ELECTR module

MT number	Class of data
507	Collisional stopping power
508	Radiative (bremsstrahlung) stopping power
501	Total
525	Large angle elastic collision ($\mu < 0.999999$)
527	Bremsstrahlung
534–572	Impact electroionization and relaxation production
530	Energy deposition by electrons
531	Charge deposition by electrons

Flow chart of electroatomic interactions

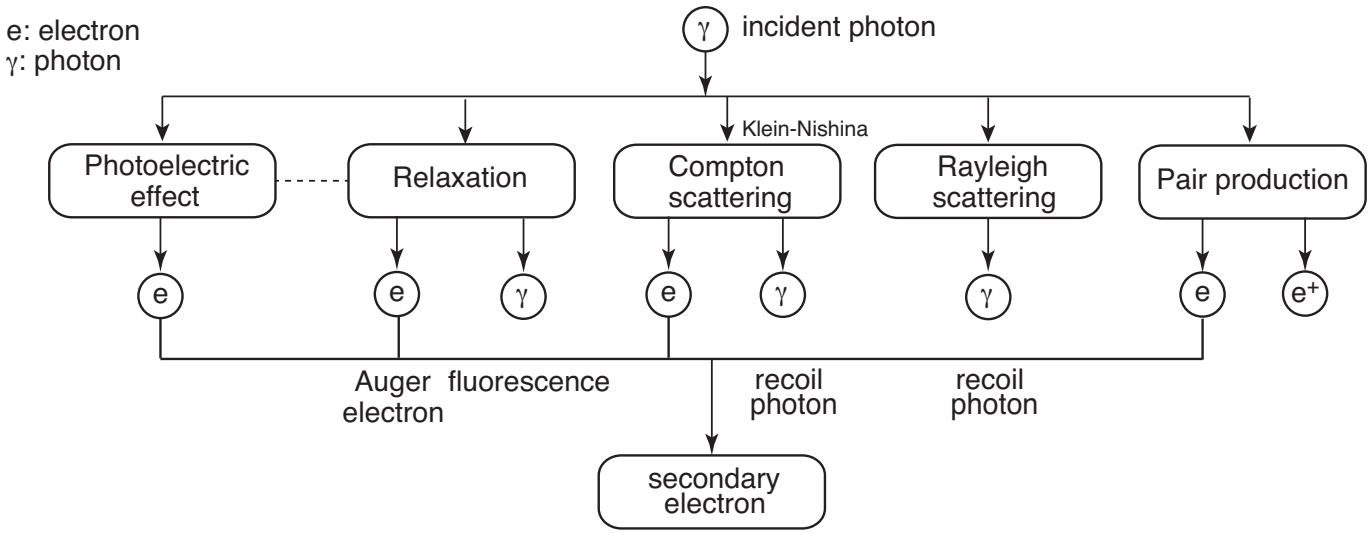


Coupled sets

- Photoatomic cross section data is generated using the GAMINR module

MT number	Data type
501	Total
502	Rayleigh scattering
504	Compton scattering
516	Pair production
522	Photoelectric effect

Flow chart of photoatomic interactions



Soft/catastrophic interactions

- Electrons lose a small amount of their energy with each collision
  - To slow down from 500 to 250 keV, an electron will undergo 4000 elastic scatterings in an aluminum foil ($Z = 13$), against 7000 in a gold foil ($Z = 79$).
  - We use the continuous slowing down model (CSDA) to describe a slowing down of all so-called soft interactions involving secondary electrons with energy below a threshold E_s.
- the *microscopic stopping power* $s(E)$ is the average rate at which the electrons lose energy at any point along their tracks, according to

$$s(E) = -\frac{1}{N}\frac{dE}{dx} \tag{1}$$

where N is the number of atoms per unit volume.
- The stopping power represents components of atomic excitation, inelastic collision and bremsstrahlung processes. The stopping power is evaluated data, in units of Mev-barn, formally defined by the relation

$$s(E) = \int_{E_{\min}}^{E} dE' \, (E - E') \, \sigma(E \to E') \tag{2}$$

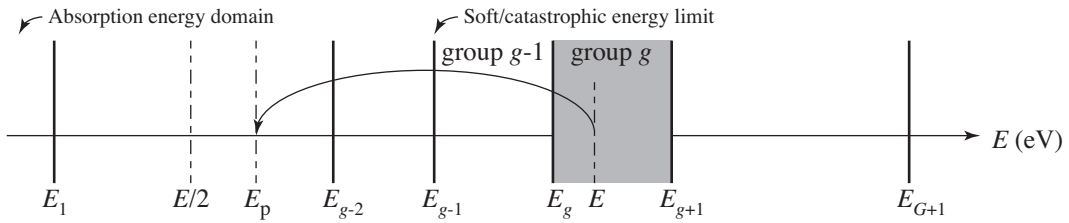
keeping in mind that $\sigma(E \to 0)$ or $\sigma(E \to E)$ may diverge.

Soft/catastrophic interactions

- According to CEPXS, the lower energy limit $E_{\min}$ is set to $E/2$ for the collisional stopping power and to 1 Kev for radiative stopping power:

$$s^{\text{col}}(E) = \int_{E/2}^{E} dE' \, (E - E') \, \sigma_{\text{col}}(E \to E') \, . \tag{3}$$

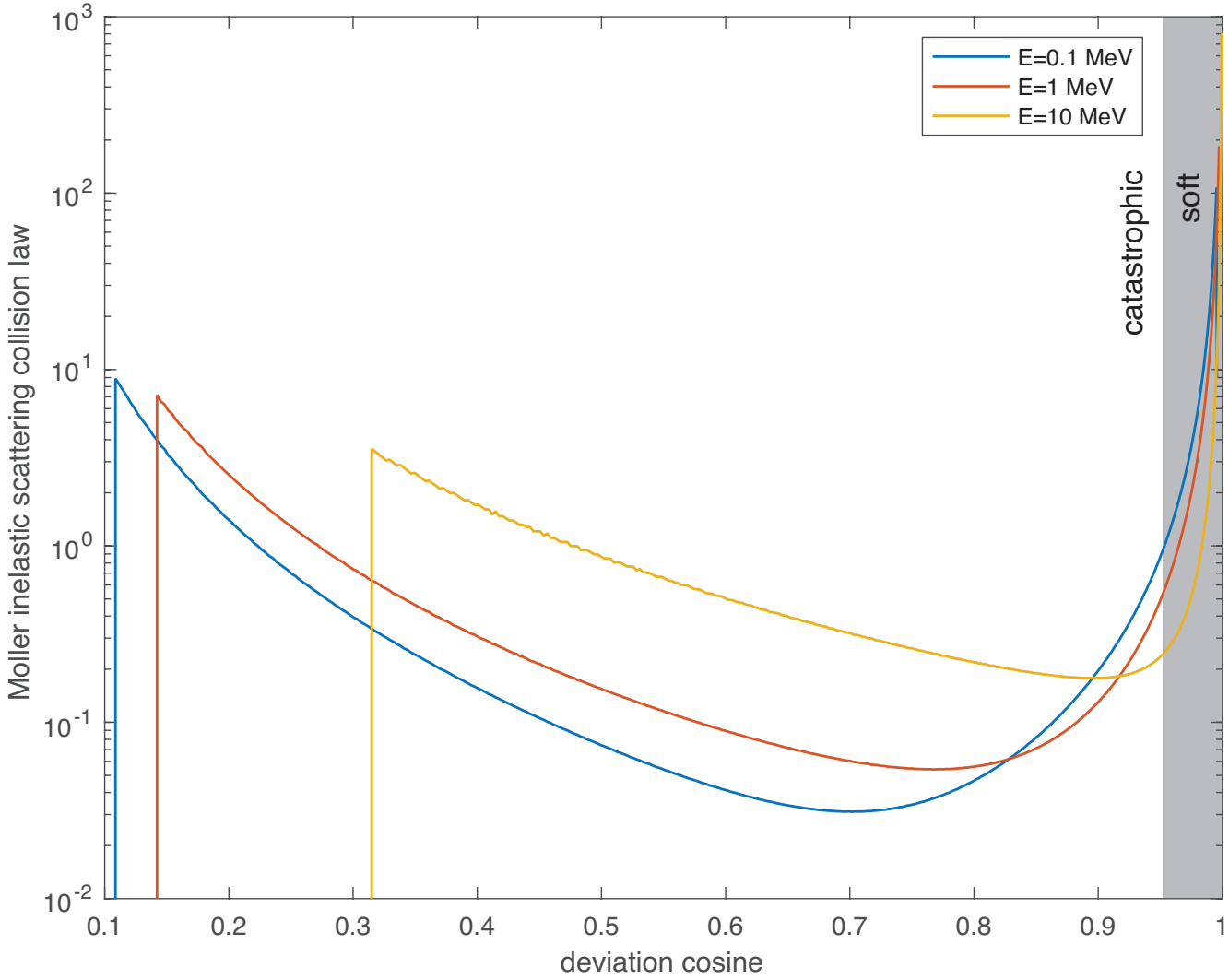
- A BFP solution of the electroatomic transport equation consists to use:
  - the CSDA equation in the soft energy domain
  - the Boltzmann equation in the catastrophic energy domain.
- A discretization of the group G is defined in energy, as illustrated in the figure. Each group g is defined with limits between E_g and E_{g+1}.



- The energies $E < E_1$ correspond to the absorption domain.
- The energy E_{g-1} corresponds to the boundary between the soft and catastrophic domains.

Soft/catastrophic interactions

- The Moller law can be used to represent inelastic collisions without relaxation
- The forward peaked scattering is represented as soft interaction.



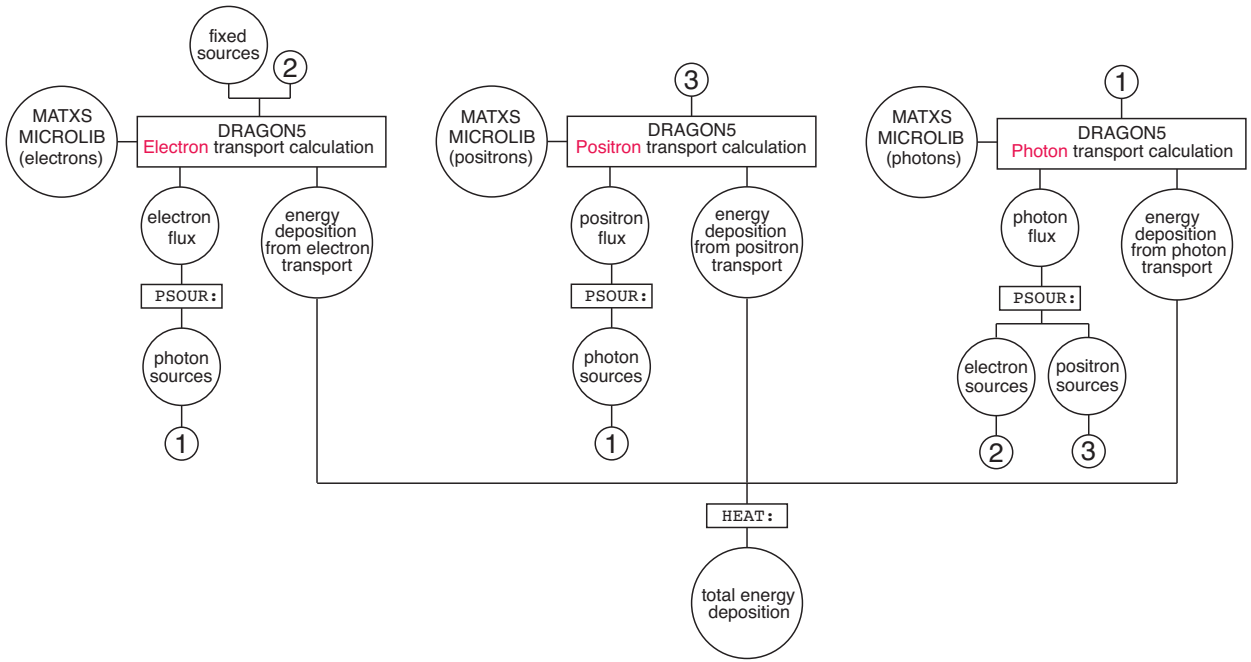
Solution of the BFP equation

- The BFP equation represents the transport of electrons and positrons. In this case, the term of charged particle scattering has a strong forward anisotropic component.
- We obtain a coupled system of three Boltzmann integrodifferential equations describing the fluxes of photons (ψ_1), electrons (ψ_2) and positrons (ψ_3) of the form

$$\boldsymbol{\Omega}\cdot\nabla\psi_1 + K_1\{\psi\} = Q_1, \quad \boldsymbol{\Omega}\cdot\nabla\psi_2 + K_2\{\psi\} = Q_2, \quad \boldsymbol{\Omega}\cdot\nabla\psi_3 + K_3\{\psi\} = Q_3 \tag{4}$$

with the notation $\psi \equiv (\psi_1, \psi_2, \psi_3)$, where $K_j\{\psi(\boldsymbol{r}, E, \boldsymbol{\Omega})\}$ is the scattering source and Q_j is the external source of particle j.

- The coupled set of Boltzmann and BFP equations is solved with code DRAGON5 and is based on MATXS cross-section data.



Solution of the BFP equation

- The BFP equation has an integral backward scattering operator similar to that used for photons and a forward scattering operator of the type L_{FP}.
- The scattering source for a charged particle is written

$$\begin{aligned} K_j\{\psi(\boldsymbol{r},E,\boldsymbol{\Omega})\} &= \Sigma_{\text{r},j}(\boldsymbol{r},E)\psi_j(\boldsymbol{r},E,\boldsymbol{\Omega}) - L_{\text{FP}}\{\psi_j(\boldsymbol{r},E,\boldsymbol{\Omega})\} \\ &- \frac{1}{2\pi}\int_{4\pi} d^2\Omega' \int_0^\infty dE' \sum_{j'=1}^{3} \Sigma_{\text{s},j\leftarrow j'}(\boldsymbol{r},E\leftarrow E',\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')\,\psi_{j'}(\boldsymbol{r},E',\boldsymbol{\Omega}') \end{aligned} \tag{5}$$

  where $\Sigma_{\text{r},j}$ is the restricted (or catastrophic) total macroscopic cross section of charged particles.
- The diffusion operator $K\psi$ for soft interactions is approximated by a linear differential operator L_{FP} based on a Taylor expansion, called the Fokker-Planck operator defined as

$$L_{\text{FP}}\{\psi_j(\boldsymbol{r},E,\boldsymbol{\Omega})\} = \frac{\partial}{\partial E}\left[S(\boldsymbol{r},E)\,\psi(\boldsymbol{r},\boldsymbol{\Omega},E)\right] \tag{6}$$

  where $S(\boldsymbol{r},E)$ is the macroscopic stopping power (MeV/cm).
- The Sternheimer density correction for charged particles is implemented in the `LIB:` module of DRAGON5.
- Equations (4) solution is currently based on the discrete ordinates method (S_n) in DRAGON5 using high order diamond differencing (HODD) or discontinuous Galarkin (DG) discretization in space.

Solution of the BFP equation

- Calculation of the energy deposition and dose made by each particle population is required to build the global computational scheme.
- Additional modules will be implemented in DRAGON5 to produce the required information:

`PSOUR:` Set the right-hand-side source term in the BTE or BFP equation originating from companion particles. This module is called three times in the DRAGON5 computational scheme.

`HEAT:` Add components of energy deposition from photoatomic and electroatomic and compute the dose.

Conclusion

- The ELECTR module is dedicated to the production of multigroup electroatomic cross-sections for use in deterministic solutions of the BFP equation.
- Availability of module ELECTR is a long-standing request from NJOY community.
- ELECTR with ENDF mode is an Open-Source contribution distributed under the BSD license.
- The actual implementation is a beta version requiring further validation.
  - The state of validation of ELECTR (CEPXS mode) at Polytechnique Montréal will be presented by Ahmed Naceur in the next talk.
  - An issue remains to be corrected with the ENDF mode. Collaboration is welcome.
- The source code of ELECTR (ENDF mode) is available at `http://merlin.polymtl.ca/pynjoy2012.htm`.

Ressources

- Academic:
  Alain Hébert (alain.hebert@polymtl.ca)
  Ahmed Naceur (ahmed.naceur@kinectrics.com)
- PyNjoy 2012 website:
  `http://merlin.polymtl.ca/pynjoy2012.htm`
- DRAGON5 website:
  `http://merlin.polymtl.ca/version5.htm`
- Textbook:
  Alain Hébert, Applied Reactor Physics,
  Presses Internationales Polytechnique,
  Third edition, Montréal, 2020.
  (to order)